

Environmental Assessment and Risk Analysis Element



Research Project Summary



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A SCREENING MODEL FOR PREDICTING CONCENTRATIONS OF VOLATILE ORGANIC CHEMICALS IN SHOWER STALL AIR

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Abstract

A simple equilibrium model was developed to predict maximum possible concentrations of volatile organic chemicals that may occur in shower stall air from the use of contaminated water during a showering event. The only site-specific parameter that must be known to use the model is the contaminant concentration in the influent water. Data was compiled from four previous studies for which vapor concentrations of contaminants in experimental shower stalls were measured. Peak concentrations reported in these experiments were compared to model-predicted concentrations. Experimental peak concentrations were typically within an order magnitude of concentrations predicted from the model (used under standard conditions), with the predicted value almost always being the higher of the two concentrations. When the model-predicted values were adjusted for experimentally reported values for water temperature, air exchange rates, and water flow rates, agreement between experimental and predicted values improved; predicted values usually were in the range of 1 to 3 times the experimental peak concentrations. The behavior of the model suggests that it would be useful as a screening tool for estimating maximum concentrations of volatile organic chemicals in shower stall air, arising from the use of contaminated water during a showering event. Example calculations of shower water criteria to protect against unacceptable inhalation exposures indicated that at times these criteria were lower than drinking water Maximum Contaminant Levels or other criteria based on ingestion of the water. This research was supported through the New Jersey A-280 Drinking Water Research Fund.

Introduction

During the past decade, increasing attention has been given to the potential for significant inhalation exposures to volatile organic chemicals (VOCs) during showering (Moya et al., 1999; Keating et al., 1997; Giardino and Andelman, 1996; Weisel and Jo, 1996; Tancrede et al., 1992). Requests for assessments of this exposure pathway have become more frequent at the NJDEP as awareness of its potential importance has increased. While residents of dwellings with VOC-contaminated water may be instructed to drink bottled water until a water treatment system is installed, it has also been necessary to make rapid decisions as to whether or not contaminated water may be used in the meantime for other purposes, such as for showering. This decision usually must be made when only one piece of information is known: the concentration of the VOC in the influent shower water.

Models that evaluate the potential inhalation of VOCs during showering have been evolving as the kinetics of contaminant volatilization from shower systems has become better understood (Moya et al., 1999; Little, 1992; McKone, 1987; Wilkes et al., 1996). While some of these approaches may be recommended for more advanced analysis, they are too complex for routine use as a screening tool. For screening purposes, a rapid, simple assessment of maximum contaminant concentrations that may be encountered in shower stall air is desired. In this study, a simple

equilibrium model has been developed to calculate a conservative estimate of the maximum concentration of a VOC that might be observed in shower stall air as a function of its concentration in the influent water.

Methods

Screening Model

The screening model was derived from the expression for the dimensionless form of the Henry's law constant, and calculates the equilibrium contaminant concentration in air (C_{air}) from of known concentration in influent shower water (C_{water}):

$$C_{air} = C_{water} \frac{HV_{water}}{HV_{air} + V_{Water}} \quad (1)$$

where V_{air} is the volume of the shower stall, with the option of including the total volume of air exchanged from the stall during the shower event, V_{water} is the total volume of water used during a showering event, and H is the dimensionless Henry's law constant at the temperature of the shower water. This model simply calculates the equilibrium partitioning

between shower stall air and shower water and ignores contaminant exiting the system via the shower drain or air exchange.

Calculation of equilibrium air concentrations

Using Equation 1 and reported influent contaminant concentrations from experimental studies, equilibrium air concentrations were calculated for chloroform, trichloroethene, ethylbenzene, toluene, cyclohexane, ethyl acetate, and acetone. Concentrations were calculated in two ways: 1) using standard values for all input parameters except for the influent VOC concentration in water, and 2) additionally adjusting V_{air} , V_{water} and H for the total air exchanged, total water consumed, and the actual water temperatures reported by the investigators. The standard values for the model parameters were as follows: shower stall volume, 1.5 m³, no air exchange; shower water volume, 0.1 m³ (10 minute shower duration with a 10 L/minute shower flow rate); shower water temperature for calculating the Henry's law constant, 40°C. Relative to the reported studies, the shower stall volume was typical, the water temperature was equal to or above most temperatures, and the flow rate was a typical maximum value. Henry's law constants were calculated using temperature-dependant relationships for this parameter reported in recent research. The U. S. Geological Survey has conveniently summarized experimentally determined temperature-dependant relationships for the Henry's law constant for many VOCs (Rathbun, 1998).

Experimental Shower Systems

Data was extracted from four recent studies employing experimental shower systems for which contaminant concentrations in the shower stall air were directly measured (Moya et al., 1999; Keating et al., 1997; Giardino and Andelman, 1996; Jo et al., 1990). Peak contaminant concentrations were used for comparison to the screening model (except for results from Jo et al. (1990), who reported time-averaged air concentrations). The experimental conditions for these studies varied widely with regard to shower stall air exchange rates (0-379 L/min), shower water temperatures (19-46°C) and contaminant concentrations in the influent shower water (Table 1). Values for V_{air} and V_{water} were calculated from reported shower stall volumes, air exchange rates, water flow rates, and shower duration times.

Results

Experimentally measured contaminant concentrations in shower air were compared to predicted concentrations for eighty-nine reported experiments from four investigators, a subset of which are listed here (Table 1). Differences between the calculated and measured concentrations are reported as the ratio of the two values for convenience. A statistical summary of the ratio values was also prepared (Table 2). The experimental concentrations of Jo et al. were time-averaged, rather than peak values. The statistical summary was therefore calculated both with and without those experiments.

The most striking observation that can be made is the

relatively close agreement between concentrations predicted with the screening model and the experimentally determined peak concentrations. When screening model calculations were adjusted for experimentally reported values for V_{air} , V_{water} and water temperature, the average ratio of predicted concentrations to measured peak concentrations was less than three (Table 2). This ratio was reduced to less than two when the time-averaged data of Jo et al. was removed from the data set. When the ratios were determined using standard shower conditions, the mean ratio was approximately seven either with or without the data set of Jo et al. (Table 2).

Predicted concentrations were generally higher than measured results; the reason for this lies in the formulation of the screening model as a simple equilibrium system. The model does not account for the kinetics of contaminant volatilization or its loss from the shower system via air exchange and water exiting the shower drain. The entire mass of contaminant entering the system during the shower run is simply partitioned between the air and water phase under equilibrium conditions. Thus, a conservative (high) prediction of contaminant concentrations would be expected. Such a conservative prediction is desirable in a screening model, as long as the prediction is not unreasonably high. A commonly employed standard for a screening model is that it should give an order-of-magnitude estimate of actual contaminant concentrations. This condition was always met when the calculation was adjusted for experimental V_{air} , V_{water} and water temperature values. Even when run under standard conditions, this order of magnitude agreement was achieved more than 80% of the time, and the highest ratios were still not excessively high (between 20 and 30 for some of the cyclohexane experiments).

Another desirable feature of a screening model is that it should not under predict experimental concentrations. When run under standard conditions, the model under predicted experimentally measured concentrations only 4 times out of 89 experiments, and in those four cases the under prediction was less than a factor of two. Use of the model with experimentally adjusted values for V_{air} , V_{water} and temperature yielded predictions for 6 of 89 experiments that were between 58 and 80% of the measured values. An additional 12 predictions were only marginally low (between 80% and 100% of the measured values). While the under prediction was again less than a factor of two in all cases, it would be somewhat more prudent to calculate concentrations using standard conditions. This is also recommended for another reason: values for V_{air} , V_{water} and water temperature are not known for actual cases without site-specific investigation. The somewhat greater over prediction of peak shower concentration that results is not excessive (a factor of seven, on average).

Discussion

A simple rearrangement of Equation 1 may be used to predict acceptable influent water concentrations from an allowed air concentration in the shower stall. The latter concentration is calculated from the inhalation toxicity endpoint selected by the user and the inhalation exposure time assumed, and it is substituted for the estimated peak air concentration, C_{air} , from Equation (1). For noncarcinogens, the acceptable water concentration is

$$C_{water} = RfC \frac{1440}{10} \frac{HV_{air} + V_{water}}{HV_{water}} \quad (2)$$

where R/C is the inhalation reference concentration, and the ratio of 1440/10 is an adjustment made for the dose that would normally be received over 24 hours (1440 minutes) being concentrated into a 10 minute shower exposure time period. For carcinogens, the equivalent equation is

$$C_{\text{water}} = \frac{10^{-6} \cdot 1440 \cdot HV_{\text{air}} + V_{\text{water}}}{URF \cdot 10 \cdot HV_{\text{water}}} \quad (3)$$

where 10^{-6} is the acceptable risk level and URF is the inhalation unit risk factor. It has been estimated that dermal exposure may be roughly equivalent to inhalation exposure during a showering event (Jo et al., 1990). Incorporating this assumption into the calculation of an acceptable water concentration would require dividing the result from Equations (3) and (4) by a factor of two.

Example shower water criteria for selected VOCs to protect against unacceptable inhalation exposures are listed in Tables 3 and 4. Table 3 lists six noncarcinogens of potential concern, and Table 4 lists five carcinogens. Also shown in these tables are current New Jersey groundwater health criteria, based on ingestion of groundwater, and Maximum Contaminant Levels (MCLs) for several of the chemicals in drinking water. Henry's law constants at 40°C for these calculations were determined using a software package available from the Environmental Protection Agency (USEPA, 2000).

If dermal adsorption is ignored, the shower water criteria shown for the example noncarcinogens are all higher than the New Jersey groundwater criteria and/or MCLs (Table 3). When adjustment is made for dermal adsorption, the criteria for cis- and trans-1,2-dichloroethene fall slightly lower than the criteria based on adsorption, but overall the shower inhalation pathway for these chemicals is not a significant concern relative to the ingestion pathway. For the example carcinogens, shower water criteria were usually lower than the corresponding MCL values and the groundwater health criteria, particularly if the criteria were adjusted for dermal exposure during showering (Table 4). Of particular note is chloroform, which does not have an MCL but does have a groundwater criterion of 70 µg/L based on ingestion. The shower water criteria for chloroform of 0.12 µg/L (0.06 µg/L with adjustment for dermal exposure) is substantially lower than the groundwater criteria and suggests that the showering exposure pathway may be worthy of further consideration for some chemicals when VOCs are regulated in potable water.

The results of this study suggest that the simple model described may serve as a useful and reasonably conservative screening tool for deciding whether or not potential inhalation exposures resulting from VOC-contaminated shower water are significant relative to other exposure pathways such as ingestion. For site-specific cases, the model may suggest whether the inhalation exposure pathway warrants further investigation. For follow-up site-specific investigation, either on-site measurements or alternatively, more sophisticated models, such as the two-film model approach, described by Little and Moya et al., are recommended.

References

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Experimental data

Contaminant	Investigator	Expt. No.	Time of shower (min)	Influent			Peak concentration in shower air (Mg/M ³)	Air concentrations from model (mg/m ³)		Ratio of calculated to experimental concentrations	
				water temperature (°C)	concentration (mg/L)	V _{air} (M ³)		Adjusted conditions ^b	Standard conditions ^c	Adjusted conditions ^b	Standard conditions ^c
Chloroform	Keating et al. (1997)	1	10	35	57	630	506	3090	0.8	4.9	
		2	10	45	58.7	780	529	3183	0.7	4.1	
		5	10	40	55.6	430	498	3014	1.2	7.0	
	Giardino and Andelman (1996)	11	11.1	42	0.582	16	13	32	0.8	2.0	
		12	11.1	27	0.555	7.7	7	30	0.9	3.9	
		13	11.1	28	0.677	24.9	31	37	1.2	1.5	
	Jo et al. (1990)	1	10	40	0.0129	0.0692 ^d	0.6	0.7	8.3	10.1	
		2	10	40	0.013	0.0581 ^d	0.6	0.7	9.9	12.1	
		3	10	40	0.02	0.1242 ^d	0.9	1.1	7.1	8.7	
	Trichloroethene	Giardino and Andelman (1996)	4	10	40	0.021	0.897 ^d	0.9	1.1	1.0	1.3
			5	10	40	0.0228	0.899 ^d	1.0	1.2	1.1	1.4
			2	21.7	22	0.959	14.3	14	58	1.0	4.1
			3	18.6	21	0.493	42.8	36	30	0.8	0.7
5			18.6	46	0.922	41.9	27	56	0.7	1.3	
6			18.6	44	0.589	13.7	8	36	0.6	2.6	
7			18.6	33	0.519	54.9	41	31	0.7	0.6	
Cyclohexane	Moya et al. (1999)	8	18.6	32	0.875	33	27	53	0.8	1.6	
		1	8	0.073	6.9	28	119	4.1	17.3		
		3	8	21	3.1	7.9	33	205	4.2	26.0	
Ethylbenzene	Moya et al. (1999)	5	8	35	2.6	9.3	40	172	4.3	18.5	
		7	8	36	1.9	6.3	20	126	3.2	20.0	
		1	8	0.073	29	91	368	3.1	12.7		
		3	8	21	7.5	26	77	453	3.0	17.4	
		5	8	35	8	35	120	483	3.4	13.8	
		7	8	36	5.2	30	54	314	1.8	10.5	
		1	8	0.073	41	66	261	1.6	6.4		
Toluene	Moya et al. (1999)	3	8	21	7	34	72	406	2.1	11.9	
		5	8	35	6.4	56	95	371	1.7	6.6	
		7	8	36	5.6	47	58	325	1.2	6.9	
Ethyl acetate	Moya et al. (1999)	1	8	0.073	68	87	219	1.3	3.2		
		3	8	21	25.8	57	78	215	1.4	3.8	
		5	8	35	24.4	130	125	204	1.0	1.6	
Acetone	Moya et al. (1999)	7	8	36	23.6	81	108	197	1.3	2.4	
		1	8	0.073	36	36	105	1.0	2.9		
		3	8	21	42	35	38	116	1.1	3.3	
		5	8	35	41.6	77	80	115	1.0	1.5	
		7	8	36	41.1	71	79	113	1.1	1.6	

^a Experimental contaminant concentrations in air are peak values measured unless otherwise noted. Total number of experiments = 89.

^b V_{water} , V_{air} and Henry's law constant adjusted for experimental conditions.

^c Standard conditions as described in text.

^d Experimental concentrations are average values over duration of shower runs.

Table 2. Ratio of Calculated to Experimental Contaminant Concentrations in Shower Air: Statistical Summary

	Model calculations adjusted for experimental conditions ^a		Model calculations under standard conditions ^b	
	All experimental data (n=89)	All data except Jo et al. (n=70)	All experimental data (n=89)	All data except Jo et al. (n=70)
Average ratio	2.7	1.7	7.2	7.0
Std. dev. of ratio	2.4	1.1	5.8	6.4
Ratio range	0.6-9.9	0.6-5.6	0.6-26	0.6-26

^a Experimental values for water temperature, V_{air} and V_{water}

^b Standard values for water temperature, V_{air} and V_{water} as given in text

Table 3. Acceptable VOC Concentrations in Shower Stall Water to Protect Against Unacceptable Inhalation Exposures: Noncarcinogens

Chemical	Reference	Shower Water Criteria ($\mu\text{g/L}$)		NJDEP Groundwater
	Concentration (RfC) in Air ($\mu\text{g}/\text{m}^3$) ^a	No dermal absorption	With dermal absorption	Health Criteria ^a ($\mu\text{g/L}$)
Acetone	350	19,400	9,700	700
1,1-Dichloroethane	50	130	65	50 ^b
1,2-Dichloroethene (cis)	35	93	46	70 ^b
1,2-Dichloroethene (trans)	60	140	70	100 ^b
MTBE	300	1700	850	70 ^b
Tertiary buty alcohol (TBA)	61	7,800	3,900	100

^a Current as of May, 2002

^b Equals Maximum Contaminant Level

Table 4. Acceptable VOC Concentrations in Shower Stall Water to Protect Against Unacceptable Inhalation Exposures: Carcinogens

Chemical	Unit Risk Factor (URF) in Air ($\mu\text{g}/\text{m}^3$) ^{-1a}	Shower Water Criteria ($\mu\text{g/L}$)		NJDEP Groundwater Health Criteria ^a ($\mu\text{g/L}$)	Maximum Contaminant Level (MCL) ^a ($\mu\text{g/L}$)
		No dermal absorption	With dermal absorption		
Benzene	8.3×10^{-6}	0.30	0.15	0.2	1
Carbon tetrachloride	1.5×10^{-5}	0.15	0.08	0.4	2
Chloroform	2.3×10^{-5}	0.12	0.06	70	
Trichloroethene	1.7×10^{-6}	1.38	0.69	1	1
1,1-Dichloroethene	5.0×10^{-5}	0.04	0.02	1	2

^a Current as of May, 2002

RESEARCH PROJECT SUMMARY



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